

The Hubbard model in the canonical formulation

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We describe non-relativistic fermions on the lattice (Hubbard model) in the canonical formulation using transfer matrices in fixed fermion number sectors such that the partition function becomes fully factorized in time. By analytically integrating out the auxiliary Hubbard-Stratanovich field due to the four-fermion interaction, we express the system in terms of discrete, local fermion occupation numbers which are the only remaining degrees of freedom. We show the close relation to the fermion loop and the fermion bag formulation. One can prove that in 1+1 dimension the fermion sign problem is absent. Finally, we construct improved estimators for the ground state energy, 2-point functions, and for the chemical potential.

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1. Motivation

The sign problem at finite fermion density can be understood as a manifestation of huge cancellations between different states which contribute to the partition function in a given basis. Obviously, all states are always present in the grand-canonical partition function $Z(\mu, T)$ for any values of the chemical potential μ and temperature T . However, only some states are relevant and important for the physics at specific values of μ and T and contribute significantly to $Z(\mu, T)$, while all other states either have negligible weights or need to cancel out. A prominent example is given by the so-called Silver Blaze property of physical systems: certain physical states are completely invisible in the physical properties of the system up to the critical chemical potential μ_c , when they suddenly become the main physical degrees of freedom driving the physics.

In the canonical formulation, fewer cancellations are necessary to describe the same physics, as compared to the grand-canonical formulation. This becomes clear by considering the dimension of the Fock space. Consider for example a system specified by the Hamiltonian $\mathcal{H}(\mu)$ and its grand-canonical partition function

$$Z_{\text{GC}}(\mu, T) = \text{Tr} \left[e^{-\mathcal{H}(\mu)/T} \right] = \text{Tr} \prod_t \mathcal{T}_t(\mu),$$

where in the last step we assumed a discretized time and a Trotter decomposition, such that $\mathcal{T}_t(\mu)$ are transfer matrices at fixed time indices t . In the canonical formulation, the partition function reads

$$Z_{\text{C}}(N_f, T) = \text{Tr}_{N_f} \left[e^{-\mathcal{H}/T} \right] = \text{Tr} \prod_t \mathcal{T}_t^{(N_f)},$$

where the trace is now restricted to states with a specific fermion number N_f . As a consequence, in the canonical formulation certain cancellations are more obvious than in the grand-canonical one. In QCD, for example, the canonical partition functions vanish for the number of quarks $N_Q \neq 0 \bmod 3$ due to the transformation properties of the Fock states, while in the grand-canonical formulation the cancellation is not obvious at all. Similarly, in the $N_f = 1$ Schwinger model it is immediately obvious that in the canonical formulation only the states in the zero-charge sector are physical, because the contributions from the canonical states in the other sectors cancel due to the global $U(1)$ symmetry, while in the grand-canonical formulation the cancellation is not explicit.

The canonical transfer matrices can be constructed for a large class of quantum field theories. In some supersymmetric Yang-Mills gauge theories, for example, the canonical formulation has been shown to lead to a solution of the fermion sign problem [1, 2], based on the construction of the transfer matrices in and the close connection of the canonical formulation with the (dual) fermion loop or worldline formulation [3]. This, in turn, allows for the construction of efficient simulation algorithms, such as fermion bag [4, 5] and fermion worm algorithms [6]. Based on the construction of the canonical transfer matrices in QCD [7], one can show that the sign problem is absent in the strong coupling and heavy-dense limit, even though it is very severe just away from it. Nevertheless, in the related 3-state Potts model the sign problem at finite density can be solved by defining clusters with fixed fermion numbers in the canonical formulation [8]. In this context, it is worthwhile to note that the fermionic degrees of freedom in the canonical formulation are expressed in terms of local fermion occupation numbers $n_x = 0, 1$, and the only fermionic degrees of freedom are discrete index sets.

One can also construct improved estimators for fermionic correlation functions using the canonical transfer matrices, potentially allowing for local (multi-level) update schemes with exponential improvement of the signal-to-noise ratio, or even for the direct Monte-Carlo sampling of the correlation function. In some cases, the canonical formulation makes it possible to integrate out explicitly the (auxiliary) bosonic degrees of freedom, such as the Hubbard-Stratonovich field in the Hubbard model, thereby solving the fermion sign problem explicitly in $d = 1 + 1$ dimension.

In these proceedings, we consider the specific example of the Hubbard model and demonstrate in detail the connections and constructions mentioned above. We note that some of these ideas have been considered in the Hubbard model some time ago in [9, 10, 11, 12].

2. Canonical formulation of the Hubbard model

Let us consider the Hamiltonian for the Hubbard model,

$$\mathcal{H}(\mu) = - \sum_{\langle x,y \rangle, \sigma} t_\sigma \hat{c}_{x,\sigma}^\dagger \hat{c}_{y,\sigma} + \sum_{x,\sigma} \mu_\sigma N_{x,\sigma} + U \sum_x N_{x,\uparrow} N_{x,\downarrow},$$

where $\sigma = \downarrow, \uparrow$ denotes two fermion species, e.g., with spin up or down, $c_{x,\sigma}^\dagger$ and $c_{x,\sigma}$ are the creation and annihilation operators for the corresponding fermion at position x , while $\langle x,y \rangle$ denotes the nearest neighbours and t_σ the hopping parameter. The four-fermion interaction between the fermions is parametrized by the local particle number $N_{x,\sigma} = \hat{c}_{x,\sigma}^\dagger \hat{c}_{x,\sigma}$ and the coupling strength U , while the total particle number is tuned through the chemical potentials μ_σ .

The grand-canonical partition function can now be written as

$$Z_{\text{GC}}(\mu) = \text{Tr} \left[e^{-\mathcal{H}(\mu)/T} \right] = \sum_{\{N_\sigma\}} e^{-\sum_\sigma N_\sigma \mu_\sigma / T} \cdot Z_C(\{N_\sigma\}),$$

where in the last step we perform a fugacity expansion in order to express the grand-canonical partition function in terms of the canonical ones, i.e., $Z_C(\{N_\sigma\}) = \text{Tr} \prod_t \mathcal{T}_t^{(\{N_\sigma\})}$. Note that the canonical transfer matrices are now restricted to states with fixed total fermion number $N_\sigma = \sum_x N_{x,\sigma}$.

In order to investigate the model nonperturbatively using Monte Carlo simulations, one usually performs a Trotter decomposition and introduces a coherent state representation for the fermionic degrees of freedom, eventually yielding the partition function in terms of a path integral over Grassmann-valued fields ψ^\dagger and ψ ,

$$Z_{\text{GC}}(\mu) = \int \mathcal{D}\psi^\dagger \mathcal{D}\psi e^{-S[\psi^\dagger, \psi; \mu]},$$

with Euclidean action

$$S[\psi^\dagger, \psi; \mu] = \sum_\sigma \psi_\sigma^\dagger \nabla_t \psi_\sigma + H[\psi^\dagger, \psi; \mu],$$

where the Hamilton function H describes the spatial hoppings of the Grassmann fields as well as the four-fermion interaction. This interaction can be bilinearized by a Hubbard-Stratonovich (HS) transformation using the HS field ϕ leading to

$$Z_{\text{GC}}(\mu) = \int \mathcal{D}\psi^\dagger \mathcal{D}\psi \mathcal{D}\phi \rho[\phi] e^{-\sum_\sigma S[\psi_\sigma^\dagger, \psi_\sigma, \phi; \mu_\sigma]},$$

with the action $S[\psi_\sigma^\dagger, \psi_\sigma, \phi; \mu_\sigma] = \psi_\sigma^\dagger M[\phi; \mu_\sigma] \psi_\sigma$ now being a bilinear form in the fermion fields $\psi_\sigma^\dagger, \psi_\sigma$ involving the fermion matrix M , and $\rho[\phi]$ being the Boltzmann factor for the HS field ϕ . The fermion fields can now be integrated out, yielding the determinant of M ,

$$Z_{\text{GC}}(\mu) = \int \mathcal{D}\phi \rho[\phi] \prod_{\sigma} \det M[\phi; \mu_\sigma].$$

The HS transformation can be chosen in such a way, cf. e.g. [13], that the fermion matrix has the structure

$$M[\phi; \mu_\sigma] = \begin{pmatrix} B & 0 & \dots & \pm e^{\mu_\sigma} C(\phi_{L_t-1}) \\ -e^{\mu_\sigma} C(\phi_0) & B & \dots & 0 \\ \vdots & \ddots & \ddots & \vdots \\ 0 & \dots & -e^{\mu_\sigma} C(\phi_{L_t-2}) & B \end{pmatrix}$$

where B and C are matrices of size $L_s \times L_s$, and L_s and L_t are the number of spatial and temporal lattice points. Note that while B is a constant matrix, $C = C(\phi_t)$ only depends on the HS fields on time slice t and can be chosen diagonal. The determinant of M can be dimensionally reduced to [9]

$$\det M[\phi; \mu_\sigma] = \det B^{L_t} \cdot \det(1 \mp e^{L_t \mu_\sigma} \mathcal{T}[\phi])$$

where $\mathcal{T}[\phi] = B^{-1} C(\phi_{L_t-1}) \cdot \dots \cdot B^{-1} C(\phi_0)$. The fugacity expansion of this object yields the canonical determinants $\det M_{N_\sigma}[\phi]$ as the coefficients of the corresponding fugacity terms. They can be expressed as a sum over the principal minors $\det \mathcal{T}^{\mathcal{X}\mathcal{X}}$ of order N_σ ,

$$\det M_{N_\sigma}[\phi] = \sum_J \det \mathcal{T}^{\mathcal{X}\mathcal{X}}[\phi] = \text{Tr} \left[\prod_t \mathcal{T}_t^{(N_\sigma)}[\phi_t] \right], \quad (2.1)$$

where the index sets $J \subset \{1, \dots, L_s\}$ of size $N_\sigma = |J|$ essentially label the states of the fermion Fock space and therefore allow to identify the sum as the trace over the product of transfer matrices acting in the Fock space of states with fixed fermion number N_σ . Indeed, in sector N_σ the number of states $N_{\text{states}} = \binom{L_s}{N_\sigma}$ is equal to the number of principal minors of order N_σ . At half-filling, this number grows exponentially with L_s , however, it can efficiently be evaluated stochastically with Monte Carlo methods, as for example in [1, 2].

3. Transfer matrices of the Hubbard model

Using eq. (2.1) we can now identify the transfer matrices and write down explicit expressions for them. To this end we recall the Cauchy-Binet formula

$$\det(A \cdot B)^{\mathcal{X}\mathcal{K}} = \det A^{\mathcal{X}\mathcal{I}} \cdot \det B^{\mathcal{I}\mathcal{K}}$$

and factorize $\mathcal{T}[\phi]$ into the product of transfer matrices $\mathcal{T}_t^{(N_\sigma)}[\phi_t]$, which are hence given by

$$(\mathcal{T}_t^{(N_\sigma)})_{IK} = \det B \cdot \det[B^{-1} \cdot C(\phi_t)]^{\mathcal{X}\mathcal{K}} = \det B \cdot \det(B^{-1})^{\mathcal{X}\mathcal{I}} \cdot \det C(\phi_t)^{\mathcal{I}\mathcal{K}},$$

where $|I| = |J| = |K| = N_\sigma$. Moreover, using the complementary cofactor we have

$$\det B \cdot \det(B^{-1})^{\mathcal{X}\mathcal{I}} = (-1)^{p(I, J)} \det B^{IJ},$$

where $p(I, J) = \sum_i (I_i + J_i)$. Since the HS transformation can be chosen such that $C(\phi_t)$ is diagonal, we find

$$\det C(\phi_t)^{JK} = \delta_{JK} \prod_{x \in J} \phi_{x,t}$$

and the HS field can be integrated out site by site,

$$\int d\phi_{x,t} \rho(\phi_{x,t}) \phi_{x,t}^{\sum_{\sigma} \delta_{x \in J^\sigma}} \equiv w_{x,t} = \begin{cases} w_2, & \text{if } x \notin J^\uparrow, x \notin J^\downarrow, \\ w_1, & \text{else,} \\ w_0, & \text{if } x \in J^\uparrow, x \in J^\downarrow, \end{cases}$$

where $w_i > 0$. Finally, with $\prod_x w_{x,t} \equiv W(\{J_t^\sigma\})$ we have the canonical partition function of the Hubbard model expressed in fully factorized form,

$$Z_C(\{N_\sigma\}) = \sum_{\{J_t^\sigma\}} \prod_t \left(\prod_{\sigma} \det B^{J_{t-1}^\sigma J_t^\sigma} \right) W(\{J_t^\sigma\}), \quad |J_t^\sigma| = N_\sigma, \quad (3.1)$$

with the only dynamical degrees of freedom being the index sets $\{J_t^\sigma\}$ on each time slice. The representation in eq. (3.1) exposes the relation to the fermion loop formulation. Interpreting the spatial indices in the index sets J_t^σ as labelling the positions of the N_σ fermions where they hop in time, one can identify the N_σ fermion loops running around the lattice in temporal direction, cf. Figure 1 for an illustration with $N_\sigma = 2$ in $d = 1$ spatial dimension. The factors $\det B^{J_{t-1}^\sigma J_t^\sigma}$ collect all the contributions from different fermion loop configurations on time slice t within the shaded regions. They can therefore be interpreted as “fermion bags”. It turns out that in $d = 1$ spatial dimensions the contributions $\det B^{IJ}$ can be calculated analytically through the recursion relation [14]

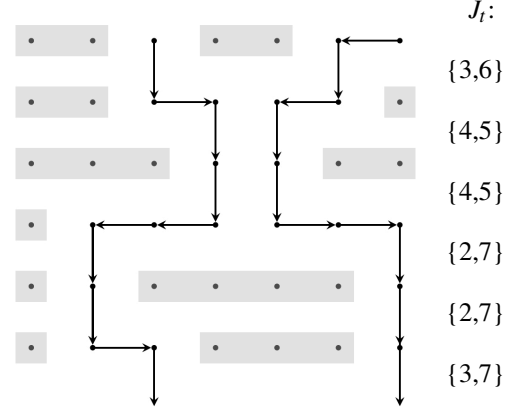


Figure 1: Illustration of a fermion loop configuration and the corresponding index sets J_t .

$$\begin{array}{c} \bullet \bullet \bullet \bullet \bullet \end{array} = \begin{array}{c} \bullet \bullet \bullet \bullet \bullet \end{array} \begin{array}{c} \circlearrowleft \end{array} + \begin{array}{c} \bullet \bullet \bullet \bullet \bullet \end{array} \begin{array}{c} \circlearrowright \end{array}$$

and for open b.c. one can prove that $\det B^{IJ} \geq 0$, i.e., there is no sign problem. For periodic b.c. there is no sign problem either, because in the thermodynamic limit, the partition functions become independent of the boundary conditions.

4. Improved estimators

Having the canonical partition function in its fully factorized form, we can construct improved estimators for various observables. The energy of the ground state, for example, is defined by $E_0 = -\lim_{\beta \rightarrow \infty} \partial_\beta \ln Z_C(\beta)$, which on the lattice becomes

$$E_0 = \lim_{L_t \rightarrow \infty} \ln \frac{Z_C(L_t)}{Z_C(L_t + 1)}.$$

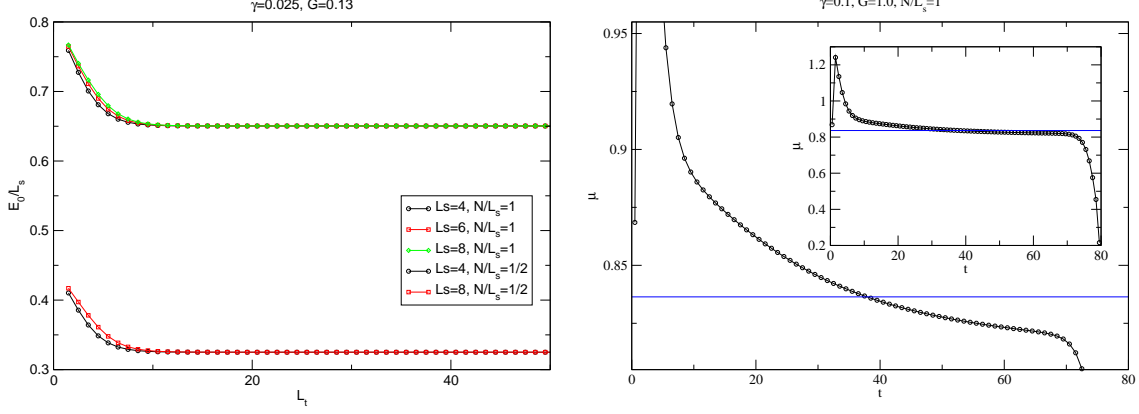


Figure 2: *Left plot:* Logarithm of the partition function ratios $Z_C(L_t)/Z_C(L_t + 1)$ as a function of L_t which yields the ground state energy E_0 in the limit $L_t \rightarrow \infty$. *Right plot:* Chemical potential from eq. (4.2) as a function of t . The blue line is the value obtained via eq. (4.1) from the ratio $Z_C(n, n_s)/Z_C(n + 1, n_s + 1)$.

Since our formulation is factorized in time, we can write the ratio as an observable calculated in the ensemble defining $Z_C(L_t + 1)$,

$$\frac{Z_C(L_t)}{Z_C(L_t + 1)} = \left\langle \prod_{\sigma} \left(\frac{\det B_{t-1}^{J_{t-1}^{\sigma} J_t^{\sigma}}}{\det B_{t-1}^{J_{t-1}^{\sigma} J_t^{\sigma}} \det B_{t-1}^{J_t^{\sigma} J_{t+1}^{\sigma}}} \right) \frac{1}{W(\{J_t^{\sigma}\})} \right\rangle_{Z_C(L_t + 1)}.$$

In the left plot of Figure 2 we show the logarithm of this ratio (normalized by the volume L_s) as a function of the inverse temperature $1/T = L_t$ for two different fermion densities $\rho = N/L_s = (N_{\uparrow} + N_{\downarrow})/L_s = 1$ (half-filling) and $1/2$ (quarter-filling) for specific values of the hopping $t_{\uparrow} = t_{\downarrow}$ and the four-fermion coupling U (parametrized by γ and G). As another example we consider the chemical potentials $\mu_{(s)}$ defined as $\mu_{(s)} = \partial_{\rho_{(s)}} F(\rho_{(s)})$ with $\rho_{(s)} = (N_{\uparrow} \pm N_{\downarrow})/L_s$ which on the lattice can be written as, e.g.,

$$\mu = \frac{F(n + 2, n_s) - F(n, n_s)}{2} = -\frac{1}{2L_t} \ln \left(\frac{Z_C(n + 2, n_s)}{Z_C(n, n_s)} \right). \quad (4.1)$$

Now we define the partition function for the fermionic 2-pt. function of, e.g., an up-spin fermion in the background of $\{N_{\sigma}\}$ fermions,

$$Z_t^{2\text{-pt}, \uparrow}(\{N_{\sigma}\}) = \text{Tr} \left[P^{\dagger} \prod_{t' < t} T_{t'}^{\{N_{\uparrow} + 1, N_{\downarrow}\}} P \cdot \prod_{t' \geq t} T_{t'}^{\{N_{\sigma}\}} \right] = \langle \langle \psi_0^{\dagger} \psi_t \rangle \rangle_{\{N_{\sigma}\}},$$

where P^{\dagger} (P) create (annihilate) an up-spin fermion at time $t' = 0$ ($t' = t$). Then we can write the chemical potential as a telescopic product of ratios of 2-pt. functions,

$$e^{-2\mu/T} = \frac{Z_0^{2\text{-pt}, \uparrow}}{Z(n, n_s)} \cdot \frac{Z_1^{2\text{-pt}, \uparrow}}{Z_0^{2\text{-pt}, \uparrow}} \cdots \frac{Z(n + 1, n_s + 1)}{Z_{L_t-1}^{2\text{-pt}, \uparrow}} \times \frac{Z_0^{2\text{-pt}, \downarrow}}{Z(n + 1, n_s + 1)} \cdot \frac{Z_1^{2\text{-pt}, \downarrow}}{Z_0^{2\text{-pt}, \downarrow}} \cdots \frac{Z(n + 2, n_s)}{Z_{L_t-1}^{2\text{-pt}, \downarrow}}.$$

Each ratio can in turn be written as an expectation value, e.g.,

$$\frac{Z_{t+1}^{2\text{-pt}, \uparrow}}{Z_t^{2\text{-pt}, \uparrow}} = \left\langle \frac{\sum_{\{J'_{t+1}\}} \det B_{t+1}^{J'_{t+1} J'_{t+1}} \cdot W(\{J'_t, J'_t\})}{\sum_{\{J_t\}} \det B_t^{J_t J_{t+1}} \cdot W(\{J_t, J_t\})} \right\rangle_{Z_t^{2\text{-pt}, \uparrow}}, \quad (4.2)$$

where $|J'_{t+1}| = |J_t| + 1 = N_\uparrow + 1$, and the chemical potential can be calculated from the logarithmic sum of the corresponding observables. In the right plot of Figure 2 we show the chemical potential for a single fermion obtained in this way. The shape of the curve depends very much on the operators P^\dagger, P , i.e., the wave function used to create and annihilate the fermion.

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